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Calculate the Binding Energy Using the Least Squares Method to Modify the Liquid Drop Model

Enas M.Y. AL-Fraha
Department of Physics/ College of Science/ University of Mosul/ Iraq

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corresponding author:
Enas M.Y. AL-Fraha
enasmohammed@uomosul.edu.iq

ABSTRACT

The current research developed a new formula for calculating the theoretical value of nuclear binding energy and comparing it with the experimental binding energy. The liquid drop model was modified to show the effect of the interconnected relationship between the dead nucleus, i.e. The region of the nucleus composed of protons and neutrons (Z=N) which are in pairs, with the surface of the nucleus which represents the levels occupied by the unpaired neutrons (N>Z) surrounding the region of the nucleus through the potential energy (X_0), which allows a clearer understanding of the nuclear structure, leading to good information in the field of applied nuclear physics. The least squares method (LSM) was used to determine the constants of the proposed formula, by creating a code using the Fortran 95 language, and the code was solved using the Gaussian method, and the constants were found for more than 400 different nuclei (even-even, even-odd, odd-odd) within the range ($2 \geq Z \geq 92$). To determine the reliability of the proposed formula, a statistical measure was used the standard deviation (σ), its accuracy in calculating the theoretical binding energy, and the standard deviation (σ=0.384) of the updated formulation of the modified liquid drop model or (MLDM).

Keywords: Binding energy, standard deviation, least squares method, modified liquid drop model.

INTRODUCTION

There have been three distinct periods in the history of nuclear physics: The discovery of the nucleus' radioactivity at the beginning, nuclear fission at the end, and the discovery of the nucleus' fundamental constituents' protons and neutrons as well as the quantum laws governing their behavior (Nesvizhevsky and Villain, 2017). Nuclear spectroscopy and nuclear models were developed during the second period, which ran from 1947 to 1969. Eventually, the theory of microscopic uniformity, which started in the 1960s, emerged, helping to explain the behavior and structure of neutrons and protons in terms of the fundamental interactions of their constituent particles, quarks, and gluons. During this time, non-classical micro-mechanisms in the nuclear structure were also identified (Ackermann and Theisen, a 2017).

The LDM, one of the most significant nuclear models to emerge during this time, was used to explain a variety of nuclear phenomena. It was predicated on a number of suppositions, such as the idea that each nucleus had an identical nuclear force and that the nuclei are composed of an incompressible material. And at equilibrium, the atomic nuclei remain spherically symmetrical under the influence of attractive nuclear forces (Albertsson, 2022).

N. Bohr and Wheeler discovered remarkable expansions of the idea of a semi-experimental mass formula, which they applied to explain nuclear fusion and determine nuclear binding energy. It is based in part on demo accounts and part on theory. It is therefore referred to as the semi-experimental mass formula (SEMF) (Bohr and Wheeler, 1939).

Numerous research articles have been done since then to improve the LDM's form. Nevertheless, the formula's fundamental structure has remained unchanged over time, even with these advancements. To bring the theoretical nuclear binding energies closer to the experimental binding energies, the semi-experimental mass formula (SEMF) has been expanded over the years either modifying the way that different coefficients' dependence on the mass number and atomic number is altered or by adding different new coefficients. The SEMF, which consists of five different types of energy components (surface, volume, asymmetry, Coulomb repulsion, and pairing term), has significantly advanced nuclear physics (Yüksel *et al*., 2021).

The SEMF, which consists of five different types of energy components (volume, surface, Coulomb repulsion, asymmetry, and pairing term), has significantly advanced nuclear physics. The mass data is updated by the parameters of energy, which are derived from experimental data on nuclear reactions. With the use of these atomic data, numerical techniques can be used to determine a new set of energy parameters for the SEMF; the least-squares method (LSM) is one of the most significant of these techniques (Ackermann and Theisen, b 2017) however, even if the LDM provides a good estimate for atomic masses and a wide range of other phenomena, it is unable to explain the emergence of magic numbers. The predicted binding energies of the LDM are less than the real binding energies of "magic nuclei.". For nickel $(^{56}_{28}Ni)$, for instance, the LDM estimates an energy 477.7 MeV, n on one the less the measured value is 484.0 MeV, and the LDM indicates that tin $(^{132}_{50}Sn)$ will have a binding energy of 1084 MeV, while the actual value is 1110 MeV. Over the last few decades, various research publications have been dedicated to enhancing the shape of the LDM (Ryssens *et al,* 2019). The researchers UVS and Lakshminarayana, developed the LDM to find the nuclei's nuclear binding energy, and they fitted the constants of the SEMF to the LDM using the LSM, then their results were compared with the results of the original LDM and they got the rate of errors not exceeding 1.64% (UVS and Lakshminarayana, 2015), Mavrodiev, the researcher, provided a generalization of the SEMF that starting with Z=1 and N=1, characterizes for 2,654 nuclei in the AME2012 nuclear database, the measured nuclear mass values with an accuracy of less than 2.2 MeV (Mavrodiev, 2016).

Nine protons (2, 8, 14, 20, 28, 50, 82, 108, 124) and ten neutrons (2, 8, 14, 20, 28, 50, 82, 124, 152, 202) were found to have an impact. The nuclear binding energies were determined by Ankita and Suthar, two researchers, utilizing the SEMF and various constants supplied by other

researchers. Additionally, they contrasted the computed values with the results of the experiment. To identify appropriate constants using the error plot, a comparative analysis was implemented.

The study was prolonged to determine the ideal constant to lower the error (Ankita and Suthar, 2016). When the researchers UVS and Lakshminarayana compared their findings with experimental values, they demonstrated a very satisfactory agreement. To comprehend nuclear stability and nuclear binding energy in terms of strong nuclear interaction and mass difference for a broad range of light, medium, and heavy nuclei, the researchers worked on constructing the LDM in a novel approach (UVS and Lakshminarayana, 2017).

The researcher Vahid and his group used the LSM to calculate the coefficients (Coulomb, asymmetry, volume, and surface) in the SEMF for the LDM for 22 nuclei (odd-even). Then their results were compared with the results of similar previous work (Vahid *et al*., 2016). To provide the mass formula with a new set of energy parameters, researcher Benzaid, and his team updated the SEMF for mass with five energy terms and used LSM for the binding energy of 2,497 distinct nuclides from the most recent update to estimate the atomic mass. They contrasted their findings with those of related earlier research (Benzaid *et al*, 2020). The investigator Pan and his team proposed a straightforward method, based on the LDM and accounting for the shell correction, to determine the energy released from a proton's radioactivity. By comparing the experimental results for 29 nuclei with the proton's radioactivity from the ground state, they were able to determine the coefficients of this formula (Pan *et al*., 2021). The importance of the current research lies in modifying the liquid drop model to show the effect of the interconnected relationship between the dead core of the nucleus when (N=Z) with the surface of the nucleus that represents levels occupied by neutrons through the potential energy (X_0). This allows a clearer understanding of the nuclear structure, which leads to good information in the field of applied nuclear physics

This research aims to calculate the nuclear binding energy to find an improved formula for the liquid drop model that will calculate the nuclear binding energy for most types of nuclei by building a computer program in Fortran that uses the matching process using the Least-Squares Method (LSM) and finding new constants.

Theoretical framework

Liquid drop model (LDM)

Von Weizsäcker devised the LDM based on the fundamental idea that the nucleus can be viewed as a drop of an incompressible substance, which comes from the about equal internal density. Strong nucleon interactions give rise to binding energy for the nucleus that is linearly associated with its mass number (the volume of the nucleus) according to the LDM. Furthermore, interactions between surface nucleons and deep nucleus nucleons are conceivable. As a result, they have a lower binding energy than the others. Additionally, the Z has a coulomb repulsion force between them, which normally reduces the nucleus's binding energy. Higher energy levels would result from increasing the number of N to the number of Z, which would negatively (Al-jomaily and Abdullateef, 2022; Frank and Nam, 2021).

The nuclear binding energy can be represented as a function of atomic number Z and mass number AB (A, Z) as follows, according to the LDM (Cui *et al.*, 2022):

$$B(A,Z) = a_v A - a_s A^{\frac{2}{3}} - a_c \frac{Z^2}{A^{\frac{1}{3}}} - a_a \frac{(\frac{A}{2}-Z)^2}{A} + a_p A^{-\frac{1}{2}} \quad \ldots\ldots\ldots\ldots\ldots\ldots (1)$$

Where $(a_v, a_s, a_c, a_a, a_\rho)$ represents the terms of volume, surface, coulomb, asymmetry, and pairing term, respectively.

Their values $(14.8, 16.8, 0.703, 28.8, 11.2)$, respectively.

Modified liquid drop model (MLDM)

It has been supposed that the nucleus consists of two regions: The core or internal region, which contains equal numbers of protons and neutrons, which are in pairs ($N = Z$). And the outer region which contains unpaired neutrons ($N > Z$). The interaction energy between pairs of nucleons will equal the pairing energy E_P. Because there will be (2Z) nucleons in the core area, the pairing energy will be:

$$E_P = \pm a_p (2Z)^{-1/2} \quad \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (2)$$

The core would be considered to be an incompressible system, comparable to the liquid drop model, and hence the volume energy E_v will be:

$$E_v = a_v (2Z) \quad \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (3)$$

Likewise, due to the existence of Z in the nucleus' core, the Coulomb energy E_C gonna be:

$$E_C = a_c \frac{Z^2}{(2Z)^{1/3}} \quad \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (4)$$

In this model proposed, we will not take into account the energies of the surface and the asymmetry because we will deal with the surface region separately and we will also have ($N = Z$) in the core region, this implies that there is no asymmetry. It remains for us to know what kind of interaction might occur between the core region of the nucleus with the surface region containing unpaired neutrons. To simplify the matter, we will work on the assumption that the reaction leads to the average potential through which each neutron moves in the (outer) region of the surface. This will be close to what is required by the Hartree-Fock theory (Jiménez-Hoyos *et al.*, 2012). Thus, if the average voltage per neutron is denoted by x_O, then the total potential energy $B_{tot}(A, Z)$ will be - $X_O(N - Z)$; to denote this by Ep, we write (KK *et al.*, 2020).

$$E_p = -x_O(N - Z) = -x_O(A - 2Z) \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots (5)$$

By merging (2,3,4,5) equations, we will get

$$B_{tot}(A, Z) = a_v(2Z) - a_c \frac{Z^2}{(2Z)^{1/3}} - x_O(A - 2Z) + a_p (2Z)^{-1/2} \dots (6)$$

Equation (5) represents the new formula for the nuclear binding energy according to the proposed model, it should be noted that the MLDM, will be used to represent the question above. (a_v, a_c, x_O, a_ρ) represents the coefficients of the volume, coulomb, average potential, and pairing. As it is known, all the coefficients in the equation are known except for the value of the x_O, and we will get new values for all the coefficients in the above equation through LSM.

Least-squares method (LSM)

The LSM's foundation is cutting down on mistake $\mathcal{E}$ (Noon, 2022; Ahmed *et al.*, 2022) in the LDM's coefficient calculations for surface, Coulomb, volume, pairing, and asymmetry, particularly when incorporating newly discovered nuclei or treating other nuclei as extensions of super-mass nuclei. The following equation represents the following equation represents the quantity $\mathcal{E}$:

$$\mathcal{E} = \sum_{i} \left(y_i - B(Z_I, A_i)\right)^2 \quad = = \quad \sum_{i} \left(y_i - Bi(a_v, a_c, x_O, a_\rho)\right)^2 \ldots (7)$$

Where y_i is an empirical value for the nucleus's binding energy, and B_i is the hypothetical binding energy that equation (1) gives us. Stated differently; by minimizing the function E, it is possible to obtain the coefficients of volume, surface, Coulomb, asymmetry, and pairing. Stated otherwise, the initial derivative of the system needs to be zero.

$$\frac{\partial \mathcal{E}}{\partial a_v} = 0, \quad \frac{\partial \mathcal{E}}{\partial a_c} = 0, \quad \frac{\partial \mathcal{E}}{\partial x_0} = 0, \quad \frac{\partial \mathcal{E}}{\partial a_\rho} = 0 \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (8)$$

Through equation (8), we get the matrix equation (9).

$$\begin{bmatrix} +\sum_i (2Z_i)^2 & -\sum_i \frac{Z_i^{\,2}}{(2Z_i)^{-2/3}} & -\sum_i (A_i - 2Z_i)(2Z_i) & +\sum_i (2Z_i)^{1/2} \\ +\sum_i \frac{Z_i^{\,2}}{(2Z_i)^{-2/3}} & -\sum_i \frac{Z_i^{\,4}}{(2Z_i)^{2/3}} & -\sum_i \frac{(A_i - 2Z_i)Z_i^{\,2}}{(2Z_i)^{1/3}} & +\sum_i \frac{Z_i^{\,2}}{(2Z_i)^{5/6}} \\ +\sum_i (A_i - 2Z_i)(2Z_i) & -\sum_i \frac{(A_i - 2Z_i)Z_i^{\,2}}{(2Z_i)^{1/3}} & -\sum_i (A_i - 2Z_i)^2 & +\sum_i \frac{(A_i - 2Z_i)}{(2Z_i)^{1/2}} \\ +\sum_i (2Z_i)^{1/2} & -\sum_i \frac{Z_i^{\,2}}{(2Z_i)^{5/6}} & -\sum_i \frac{(A_i - 2Z_i)}{(2Z_i)^{1/2}} & +\sum_i (2Z_i) \end{bmatrix}$$

$$\begin{bmatrix} a_v \\ a_c \\ X_o \\ a_p \end{bmatrix} = \begin{bmatrix} \sum_i y_i (2Z_i) \\ \sum_i y_i \frac{Z_i^{\,2}}{(2Z_i)^{1/3}} \\ \sum_i y_i (A_i - 2Z_i) \\ \sum_i y_i (2Z_i)^{-1/2} \end{bmatrix} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (9)$$

The matrix equations mentioned above are a collection of linear equations with four variables that are solved using the Gauss technique using a Fortran 95 computer application. The algorithm is composed of three steps: The first is to input the information contained in a file, the second is to estimate the system's different parameters, and the third is to solve it using the Gauss method. The volume, Coulomb, mean voltage, and pairing terms have been tabulated in the proposed new MLDM formula. Equation (10) for the MLDM model illustrates the findings of this approach, and the MLDM equation takes on the following form:

$$B_{tot}(A,Z) = 9.5(2Z) - 0.015\frac{Z^2}{(2Z)^{1/3}} - 0.17(A-2Z) \pm 9.9(2Z)^{-1/2} \ldots (10)$$

The above formula, when applied to all the nuclei under investigation, revealed a highly respectable degree of agreement between the experimental and theoretical values, especially for heavy nuclei, and with a very acceptable standard deviation of 0.384.

Determine the standard deviation

The standard deviation was computed to assess equation (10) and compare the results with the experimental findings (Qasim and Al-jomaily, 2020).

$$\sigma = \sum_{i=1}^{N} \frac{|B_{Eexp} - B_{Etheo}|}{i} \ldots (11)$$

BE_{exp}: Indicating experimental values.

BE_{theo}: Indicating to theoretical values.

RESULTS AND DISCUSSION

Fig. (1) shows the difference between the experimental and theoretical values of nuclear binding energy and the relationship of this difference with the mass number A of MLDM, for nuclei in the range (2 ≥ Z ≥ 92) under study.

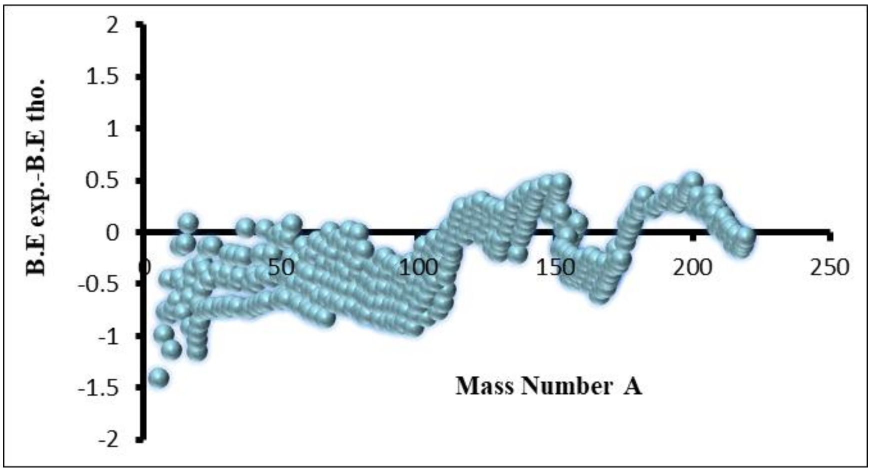

Fig. 1: The relationship between A and the difference between the theoretical and experimental binding energy.

From the figure above, we notice that the closer the difference between the theoretical and experimental values, the greater the probability of adopting the model. It is also clear that the difference between the experimental and theoretical values fluctuates around zero, which indicates the validity of the results, especially for medium and heavy nuclei, while the discrepancy between the theoretical and actual values is greater for light nuclei, due to the presence of nuclei with magic numbers (2, 8, 20, 28) for both protons and neutrons or both, and due to their closed nuclear shells, these nuclei are more stable compared to the nuclei close to them, which makes the nuclear binding energy very high. As can be explained, the Coulomb limit has a negative sign in equation (10), and as a result, its effect is weak on light nuclei and becomes stronger when the number of protons increases relative to the number of neutrons, which leads to the convergence of the experimental and theoretical values, which encourages the adoption of the model for calculating energy.

Table 1: Shows standard deviation values and root mean square deviation of the LDM and the proposed model (MLDM).

The Model	σ	The Model	σ	Improvement rate
LDM	0.682	MLDM	0.384	44%

The standard deviation of MLDM was calculated with the proposed LDM model for the model to know the accuracy and agreement of the values of the theoretical and experimental results for the nuclei under study. As we know, the closer the results are to zero, the more reliable the model is in calculating the nuclear binding energy. (Table 1) shows the validity and acceptance of the results obtained through the development rate (44%) for the proposed model compared to the original model.

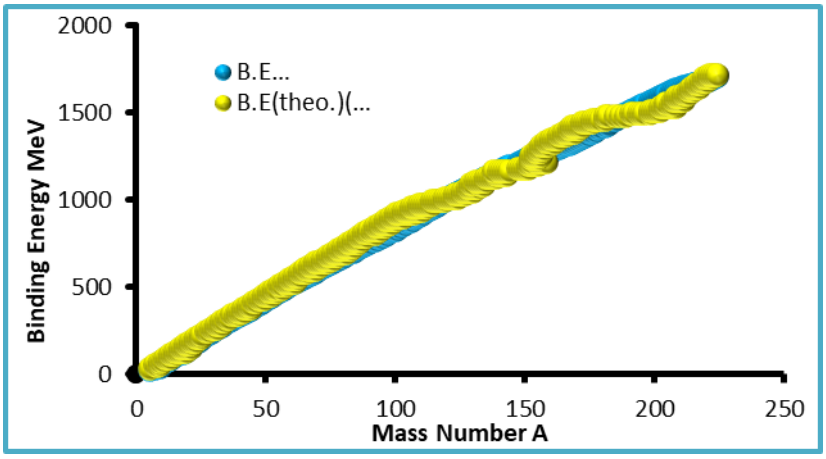

Fig. 2: A comparison of the theoretical and experimental binding energies with mass number.

Fig. (2) shows that the theoretical binding energy obtained through the new equation (11) is highly comparable to the experimental values, which indicates the accuracy of the new constants using the LSM method and supports the validity of the proposed model in estimating the nuclear binding energy. The results show that changing the number of neutrons by one unit in the surface region leads to an increase of (x_o) 30 MeV with an inverse variation and with (Z) fixed for the isotopes, while in isotopes and with (N) fixed, the potential energy (x_o) uses linearly with an increase in both (A) and (Z). It can be noted that the value of (x_o) approaches zero in nuclei in which the number of neutrons is equal to the number of protons, due to the absence of neutrons in the surface region. For nuclei with low mass, the value of (x_o) changes by a very large amount compared to the change for heavy elements due to a significant change in the ratio N/Z.

CONCLUSIONS

A modified model for determining the binding energy based on the liquid drop model was proposed, where the component coefficients were determined by fitting the least squares approach to 400 nuclei. The following conclusions can be drawn from the data.

The module MLDM, can be adopted because of the broad range of magic and non-magic nuclei that exceeded 400 nuclei.

The MLDM model gave results that showed a very satisfactory level of agreement between the theoretical and experimental values.

Statistical correlations of the standard deviation demonstrated the feasibility of using the model to calculate the nuclear binding energy.

The results showed that the proposed model outperformed the original liquid drop model in terms of the improvement rate.

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حساب طاقة الربط باستخدام طريقة المربعات الصغرى لتعديل نموذج قطرة السائل

ايناس محمد يونس الفرحة

قسم الفيزياء/ كلية العلوم/ جامعة الموصل

الملخص

طور البحث الحالي صيغة جديدة لحساب القيمة النظرية لطاقة الربط النووية ومقارنتها بطاقة الربط التجريبية. وتم تعديل نموذج قطرة السائل لإظهار تأثير العلاقة المترابطة بين النواة الميتة أي منطقة النواة المكونة من البروتونات والنيوترونات (Z=N) والتي تكون بشكل أزواج، مع سطح النواة الذي يمثل المستويات التي تشغلها النيوترونات غير المزدوجة (N>Z) المحيطة بمنطقة النواة من خلال الطاقة الكامنة (X0)، وهذا يسمح بفهم أوضح للبنية النووية، مما يؤدي إلى معلومات جيدة في مجال الفيزياء النووية التطبيقية. وتم استخدام طريقة المربعات الصغرى (LSM) لتحديد ثوابت الصيغة المقترحة، وذلك بإنشاء كود باستخدام لغة فورتران 95، وتم حل الكود باستخدام الطريقة الكاوسية، وتم إيجاد الثوابت لأكثر من 400 نواة مختلفة (زوجية–زوجية، زوجية–فردية، فردية–فردية) ضمن النطاق ($2 \leq Z \geq 92$). ولتحديد موثوقية الصيغة المقترحة تم استخدام مقياس إحصائي يسمى الانحراف المعياري (σ)، ودقته في حساب طاقة الربط النظرية، والانحراف المعياري (σ = 0.384) للصيغة المحدثة لنموذج قطرة السائل المعدل MLDM.

الكلمات الدالة: طاقة الربط، الانحراف المعياري، طريقة المربعات الصغرى، نموذج قطرة السائل المعدل.